Level crossing and quantum phase transition of the XY model

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(Dated: November 29, 2006)

Abstract

The ground state of a one-dimensional spin-1/2 chain with periodical boundary condition in the Heisenberg XY model is investigated. We consider the spatial correlation and concurrence between any nearest-neighbor pair of spins under the conditions of different coupling strength, anisotropic parameter and magnitude of a transverse field. Quantum phase transitions due to the competition between coupling and alignment which cause the abrupt changes of the correlation and concurrence are observed. The transition are direct results of the level crossing.

PACS numbers: 03.65.-w, 03.67.-a, 05.30.-d

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I. INTRODUCTION

The quantum Heisenberg XY model, which was first intensively studied by Lieb et al in the early 1960s [1], has aroused new interests in recent years. It was taken to be a potential candidate model in the practical applications in quantum computation [2, 3, 4] and quantum information [5, 6]. The Heisenberg model is not only a theoretical model with many interesting physics in it, but also realized in recent years in laboratory in physical systems such as quantum dots [7], nuclear spins [8] and electronic spins [9]. Many theoretical researchs [10, 11] had been devoted into the model to explore the important quantum properties, especially the correlation function [12], the entanglement [13] and quantum phase transition [14, 15, 16, 17, 18] in one dimensional systems. The studies show that the amount of the spatial correlation and entanglement between two spins in a spin chain (with open end) or a spin ring (with periodical boundary condition) can be modified by changing the magnitude of the external magnetic field and/or the interaction strength. And these two quantities shows singularity and obeys the scaling law in the vicinity of the quantum phase transition point of the system.

The quantum phase transition, which can take place at $T = 0$, is an interesting subject and intensively studied in the last decades [14, 19]. In this paper, we studied the quantum phase transitions of the XY model through the calculation of the correlation and the concurrence [20, 21] between two nearest-neighbor spins. By changing the magnetic field or coupling coefficient, we find that both of the two quantities have finite jumps at some critical points. The states of the system are carefully studied, the jumps are related to the level crossing [22, 23, 24] of the ground state to the excited state. The change of the symmetry of the ground state [25, 26, 27, 28, 29, 30] is the course of the quantum phase transition. The rest of this paper is organized as follows. In section II, we introduce the Hamiltonian for the Heisenberg XY model in an external field and describe the computation procedures for the correlation and the concurrence of the subsystem; Detailed results and discussions are given in section III; The conclusion of our study is given in section IV.

II. THE HAMILTONIAN AND THE THEORY

The model studied here is a one dimensional spin-1/2 chain with periodical boundary condition (PBC) [31, 32, 33] under a transverse isotropic magnetic field. The Hamiltonian is:

$$H = \sum_{i=1}^{N} (J_x \sigma_x^{(i)} \sigma_x^{(i+1)} + J_y \sigma_y^{(i)} \sigma_y^{(i+1)}) + \sum_{i=1}^{N} B_z \sigma_z^{(i)}, \tag{1}$$

where N is the number of spins, $\sigma_x^{N+1} = \sigma_x^1$ and $\sigma_y^{N+1} = \sigma_y^1$ from the PBC. J_x and J_y are the coupling strength between nearest-neighbor spins along the direction of $\vec{x}$ and $\vec{y}$, respectively, B_z is the amplitude of the magnetic field along $\vec{z}$ direction. σ_x, σ_y and σ_z are the well-known Pauli matrix:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2}$$

The parameters J_x and J_y may be represented by their average value J and anisotropic parameter γ as:

$$J_x = (1+\gamma)J, \qquad J_y = (1-\gamma)J, \tag{3}$$

and the Hamiltonian may be written as:

$$H = 2J \sum_{i=1}^{N} [(\sigma_-^{(i)} \sigma_+^{(i+1)} + \sigma_+^{(i)} \sigma_-^{(i+1)}) + \gamma(\sigma_+^{(i)} \sigma_+^{(i+1)} + \sigma_-^{(i)} \sigma_-^{(i+1)})] + \sum_{i=1}^{N} B_z \sigma_z^{(i)}, \tag{4}$$

where $\sigma_\pm = \frac{1}{2}(\sigma_x \pm i\sigma_y)$:

$$\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{5}$$

The spatial correlation [34, 35, 36] between two spins, 1 and 2, is defined by

$$C_{1,2} = \langle \sigma^{(1)} \sigma^{(2)} \rangle = \mathrm{Tr}(\rho_{12} \sigma^{(1)} \sigma^{(2)}), \tag{6}$$

$$\sigma^{(1)} \sigma^{(2)} = \sigma_x^{(1)} \otimes \sigma_x^{(2)} + \sigma_y^{(1)} \otimes \sigma_y^{(2)} + \sigma_z^{(1)} \otimes \sigma_z^{(2)}, \tag{7}$$

$$\rho_{12} = \mathrm{Tr}'(\rho). \tag{8}$$

Where $\sigma^{(1)}\sigma^{(2)}$ can be represented explicitly in a matrix form in the product eigenspace of

$\{\sigma^2, \sigma_z\}$:

$$\sigma^{(1)}\sigma^{(2)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{9}$$

And ρ_{12} is the reduced density matrix of the spin 1 and 2 derived from the density matrix ρ_S of the whole system. $\mathrm{T}r'(\cdots)$ means to trace out all the spin degrees of freedom except spins 1 and 2. In this study, we are interested in the ground state of the whole system, which is the lowest energy eigenstate ψ_0 of H, so $\rho_S = |\psi_0\rangle\langle\psi_0|$.

The concurrence of spins 1 and 2 is defined as [20, 21]:

$$Con = \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4,\ 0\}, \tag{10}$$

where λ_i are the square roots of the eigenvalues of the product matrix $\rho_{12}\tilde{\rho_{12}}$ in decreasing order. Where ρ_{12} is the reduced density matrix of the two spins subsystem, and $\tilde{\rho_{12}}$ is constructed as $(\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)$. Equation (10) applies to both of the mixed state and pure state. The reduced density matrix may be write down implicitly as:

$$\rho_{12} = \begin{pmatrix} \rho_{1,1} & \rho_{1,2} & \rho_{1,3} & \rho_{1,4} \\ \rho_{2,1} & \rho_{2,2} & \rho_{2,3} & \rho_{2,4} \\ \rho_{3,1} & \rho_{3,2} & \rho_{3,3} & \rho_{3,4} \\ \rho_{4,1} & \rho_{4,2} & \rho_{4,3} & \rho_{4,4} \end{pmatrix}, \tag{11}$$

then we get $\tilde{\rho_{12}}$ as the matrix below:

$$\tilde{\rho_{12}} = \begin{pmatrix} \rho_{4,4} & -\rho_{3,4} & -\rho_{2,4} & \rho_{1,4} \\ -\rho_{3,4}^* & \rho_{3,3} & \rho_{2,3} & -\rho_{1,3} \\ -\rho_{2,4}^* & \rho_{2,3}^* & \rho_{2,2} & -\rho_{1,2} \\ \rho_{1,4}^* & -\rho_{1,3}^* & -\rho_{1,2}^* & \rho_{1,1} \end{pmatrix}. \tag{12}$$

If the bipartite quantum state ρ_{12} is pure, it can always be written as:

$$\begin{aligned} \rho &= |\psi\rangle\langle\psi|, \\ |\psi\rangle &= a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle, \end{aligned}$$

then equation (10) could be simplified to

$$Con(|\psi\rangle) = 2|ad - bc|. \tag{13}$$

TABLE I: The discontinuities in Fig. 1

N	*J (discontinuities)*				
4	0.649	1.569	/	/	/
6	0.650	0.888	2.426	/	/
8	0.650	0.767	1.148	3.268	/
10	0.650	0.721	0.908	1.415	4.104

TABLE II: The discontinuities of the case of $N = 6$ in Fig. 2 and 4

Bz	*J (discontinuities)*		
0.65=1.30 × 0.5	*0.325*=0.650 × 0.5	*0.444*=0.888 × 0.5	*1.213*=2.426 × 0.5
1.30=1.30 × 1.0	*0.650*=0.650 × 1.0	*0.888*=0.888 × 1.0	*2.426*=2.426 × 1.0
2.60=1.30 × 2.0	*1.300*=0.650 × 2.0	*1.776*=0.888 × 2.0	*4.852*=2.426 × 2.0

III. RESULTS AND DISCUSSIONS

First, we consider the isotropic case, $\gamma = 0$, in an external field $B_z = 1.30$. Figure 1 gives the correlation functions as function of coupling strength J for different sizes of the system, ($N = 4, 6, 8, 10$). From the figures, we see that with the increase of J, C_{12} displays a "ladder" behavior. We also noted that for the case of N spins in the system, there are $N/2$ discontinuities, the position of the jump can be found in table I.

The effect of the magnitude of magnetic field on the phase transition was shown in figure 2, in which we plot the case of a 6 spins system with three different magnetic fields, $B_z = 0.65$, 1.30 and 2.6. The corresponding transition points of J are listed in table II. By simple calculation and comparison, we found that the transition values of J for each transition is approximately proportional to the magnitude of the external field.

Figure 3 plots the variation of correlation C_{12} with the applied field B_z for fixed coupling coefficient $J = 1.0$ and different values of anisotropic parameter γ. The system sizes are $N = 6$. When $|\gamma| < 0.8$, there are 3 jumps for a 6 spins system as in the case of isotropic case. However, with the increase of anisotropy γ, the magnitude of the jumps becomes smaller and the transition points moves slightly to the direction $B_z = 0$, till finally disappears in the completely anisotropic case $\gamma = 1$. Since the $\gamma = 1$ corresponding to the Ising case, where the internal number of freedom is 1, the phase transition is different to the XY case where the internal number of freedom is 2. Our calculation shows that the cross over from $n = 2$ to $n = 1$ is continuous. It is also verified that there is no quantum phase transition in the quantum Ising case.

Now we turn to the concurrence between two spins, $Con_{1,2}$. The following results were obtained for a system of $N = 6$. Figures 4 plot the variation of concurrence $Con_{1,2}$ with the coupling strength J in the isotropic case ($\gamma = 0$), the applied magnetic field fixed to three values, $B_z = 0.65$, $B_z = 1.30$ and $B_z = 2.60$. From the figures we see the same phase transition behavior as that of the correlation functions. Jumps are found at exactly the same places, which can also be checked in table II, as for the correlation functions. Figures 5 gave the variation of $Con_{1,2}$ with the magnitude of external field B_z for 8 different anisotropy γ. When $|\gamma| < 0.5$, the jumps in concurrence are clearly observed while for larger $|\gamma|$'s the magnitude of the jumps becomes smaller and smaller and turn to the smooth curve in the case of $\gamma = 1$.

It is interesting to note that the physics behind the above phase transitions turns out to be very simple and clear, it is the result of level crossing of the ground state. To clarify this point, we turn to a detailed analysis of the ground states of the system under different sets of parameters. To be specific, we use $|1\rangle$ and $|0\rangle$ to represent the "spin down" and "spin up" state for each spin in the eigenspace of $\{\sigma^2, \sigma_z\}$ respectively. The state of the whole system of N spins ψ can be written as a linear combination of 2^N states and 2^N normalized coefficients:

$$\begin{aligned} \psi &= a_0|00\cdots 00\rangle + a_1|00\cdots 01\rangle + \cdots + a_n|11\cdots 11\rangle, \\ n &= 2^N - 1, \qquad \sum_{i=0}^{n} |a_i|^2 = 1. \end{aligned} \tag{14}$$

where $|00\cdots 00\rangle$ stands for the direct product state $|0\rangle_1 \otimes \cdots |0\rangle_N$. We diagonalized the Hamiltonian and calculated the eigen function and the corresponding eigen energy. We take the coupling strength $J = 1$ and anisotropy $\gamma = 0$ for simplicity. Figure 6 shows the variation of several states energy (Someone of them will be the ground state in some interval of Bz) with the magnitude of external field B_z. It is clear from the figure that level crossing occurs at the positions where abrupt changes of the correlation function and the concurrence were observed. Concretely, when $0 < B_z \leq 0.525$, the ground state (which has been normalized) of the whole system is

$$\begin{aligned}
\psi_0^1 =& -0.11785|000111\rangle + 0.23570|001011\rangle - 0.23570|001101\rangle + 0.11785|001110\rangle \\
&- 0.23570|010011\rangle + 0.35355|010101\rangle - 0.23570|010110\rangle - 0.23570|011001\rangle \\
&+ 0.23570|011010\rangle - 0.11785|011100\rangle + 0.11785|100011\rangle - 0.23570|100101\rangle \\
&+ 0.23570|100110\rangle + 0.23570|101001\rangle - 0.35355|101010\rangle + 0.23570|101100\rangle \\
&- 0.11785|110001\rangle + 0.23570|110010\rangle - 0.23570|110100\rangle + 0.11785|111000\rangle.
\end{aligned} \tag{15}$$

Which is basically the combination of the states with antiferromagnetic order, that is, the states with half of the spins “up” and half of the spins “down”. When $0.526 \leq B_z \leq 1.464$, the ground state changed to

$$\begin{aligned}
\psi_0^2 =& +0.16667|000011\rangle - 0.28868|001001\rangle + 0.16667|001010\rangle + 0.33333|001001\rangle \\
&- 0.28868|001010\rangle + 0.16667|001100\rangle - 0.28868|010001\rangle + 0.33333|010010\rangle \\
&- 0.28868|010100\rangle + 0.16667|011000\rangle + 0.16667|100001\rangle - 0.28868|100010\rangle \\
&- 0.28868|101000\rangle + 0.16667|110000\rangle.
\end{aligned} \tag{16}$$

This is the state that 2 spins “up” and 4 spins “down”. In the course of increasing the applied field B_z, the energy level corresponding to the state (15) increases and the energy level corresponding to the state (16) decreases. At the critical field, $B_z = 0.525$, the two levels meet and then crossed, then the ground state of the spin chain is a combination of the two level states. Beyond the critical field the ground state becomes the state (16). The cross of the ground state changed the symmetry of the ground state abruptly so that a quantum phase transition occurs. At about $B_z = 1.465$, another level cross take place and over that point, the ground state of the system becomes,

$$\begin{aligned}
\psi_0^3 =& -0.40825|000001\rangle + 0.40825|000010\rangle - 0.40825|000100\rangle + 0.40825|001000\rangle \\
&-0.40825|010000\rangle + 0.40825|100000\rangle.
\end{aligned} \tag{17}$$

This is a combination of states with 1 spins “up” and 5 spins “down”. And finally, when

$B_z \geq 2.001$, the ground state is simply as

$$\psi_0^4 = |000000\rangle,$$

which is the state with ferromagnetic order. We see from the above analysis that the quantum phase transition is a result of the level crossing of the ground state, and the level crossing is simply the result of the competition between the coupling strength J, which favors antiferromagnetic order, and the applied field, which favors the ferromagnetic order. By increasing the applied field while keeping the coupling strength constant, the ground state changed from antiferromagnetic order to the ferromagnetic order in several steps, turns a spin from "up" to "down" at each step. So we observed that $\psi_0^1 \to \psi_0^2 \to \psi_0^3 \to \psi_0^4$. This also explains the number of jumps in the correlation function and concurrence, which must be half of the whole number of spins.

IV. CONCLUSION

In this paper, we studied the spatial correlation $C_{1,2}$ and the degree of entanglement $Con_{1,2}$ between two nearest-neighbor spins along a one-dimension spin ring in Heisenberg XY model. We found that in the isotropic case with fixed external field B_z, quantum phase transitions of both $C_{1,2}$ and $Con_{1,2}$ were observed with the increment of coupling strength J, the phase transitions will smoothed out as the anisotropy γ increased and disappears at the extremum value of $\gamma = 1$. The transition is a direct result of the level crossing of the ground state of the whole system, in which the symmetry of the ground state changed abruptly at the crossing point.

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[1] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys.N.Y. **16**, 407 (1961)

[2] S.B. Zheng and G.C. Guo, Phys. Rev. Lett. **85**, 2392 (2000)

[3] L. You and M.S. Chapman, Phys. Rev. A **62**, 052302 (2000)

[4] R. Raussendorf and H.J. Briegel, Phys. Rev. Lett. **86**, 5188 (2001)

[5] A. Imamoḡlu, D.D. Awschalom, et. al., Phys. Rev. Lett. **83**, 4204 (1999)

[6] G. Burkard, D. Loss and D.P. DiVincenzo Phys. Rev. B **59**, 2070 (1999)

[7] D. Loss and D.P. Divincenzo, Phys. Rev. A **57**, 120 (1998)

[8] B.E. Kane, Nature (London) **393** 133 (1998)

[9] R. Vrijen et al., e-print quant-ph/9905096

[10] K.M. O'Connor, W.K. Wootters, Phys. Rev. A **63** 052302 (2001)

[11] X. Wang, Phys. Rev. A **64** 012313 (2001)

[12] S. Liang, Phys. Rev. Lett **64** 1597 (1990)

[13] M.A. Nielson and I.L. Chuang, *Quantum Computation and Quantum Information* Cambridge University Press, Cambridge, England (2000)

[14] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press) Cambridge, England (2000)

[15] X. Peng, J.F. Du, and D. Suter, Phys. Rev. A, **71**, 012307 (2005)

[16] H.T. Quan, Z. Song, X.F. Liu, P. Zanardi, C.P. Sun, Phys. Rev. Lett., **96**, 140604 (2006)

[17] F.M. Cucchietti, S. Fernandez-Vidal, J.P. Paz, arXiv:quant-ph/0604136

[18] A.E. Allahverdyan, R. Balian and T.M. Nieuwenhuizen, Phys. Rev. A, **64**, 032108 (2001)

[19] A. Osterloh, L. Amico, et al. Nature (London) **416**, 608 (2002)

[20] S. Hill, W.K. Wootters, Phys. Rev. Lett. **78**, 5022 (1997)

[21] W.K. Wootters, Phys. Rev. Lett. **80**, 2245 (1998)

[22] S.L. Zhu, Phys. Rev. Lett., **96**, 077206 (2006)

[23] M.M. Wolf, G. Ortiz, F. Verstraete, J.I. Cirac, arXiv: cond-mat/0512180

[24] A. Langari, Phys. Rev. B, **69**, 100402 (2004)

[25] P.W. Anderson, Phys. Rev., **86**, 694 (1952)

[26] N.M. Hugenholtz and D. Pines, Phys. Rev., **116**, 489 (1959)

[27] R. Botet and R. Jullien, Phys. Rev. B, **27**, 613 (1983)

[28] Y. Aharonov and A. Casher, Phys. Rev. A, **19**, 2461 (1979)

[29] C.K. Majumdar, J. Phys. C, **3**, 911 (1970)

[30] T. Tonegawa and I. Harada, J. Phys. Soc. Jpn, **56**, 2153 (1987)

[31] H.T. Wang, Phys. Rev. B, **65**, 024426 (2002)

[32] L.G. Marland and D.D. Betts, Phys. Rev. Lett., **43**, 1618 (1979)

[33] C. Tannous, Phys. Rev. B, **32**, 4770 (1985)

[34] B.M. McCoy, E. Barouch and D.B. Abraham, Phys. Rev. A, **4**, 2331 (1971)

[35] T. Giamarchi and H.J. Schulz, Phys. Rev. B, **39**, 4620 (1989)

[36] D.P. Landau and J. Thomchick, **50**, 1822 (1979)

Figure Captions

FIG. 1: The nearest-neighbor correlation $C_{1,2}$ in different size of the spin ring as function of coupling strength J, parameters are $\gamma = 0$ and $Bz = 1.30$.

FIG. 2: The nearest-neighbor correlation $C_{1,2}$ under three different cases of external field: $B_z = 0.65$, $B_z = 1.30$ and $B_z = 2.60$, the parameter $\gamma = 0$.

FIG. 3: The dependence of nearest-neighbor correlation $C_{1,2}$ on the applied field B_z with different anisotropic parameters γ. All the results are calculated with $J = 1.0$.

FIG. 4: The comparison of Concurrence for two spins in the isotropic case, $\gamma = 0$, in three different applied field: $B_z = 0.65$, $B_z = 1.30$ and $B_z = 2.60$.

FIG. 5: The dependence of Concurrence Concurrence for two spins on the applied field B_z with different anisotropic parameters γ. All the results are calculated with $J = 1.0$.

FIG. 6: The energy levels as function of B_z for given coupling strength, the system size is $N = 6$, some of the levels which do not take part in the level crossing were omitted for clarity. The other parameters are: $\gamma = 0.0$, $J = 1.0$.

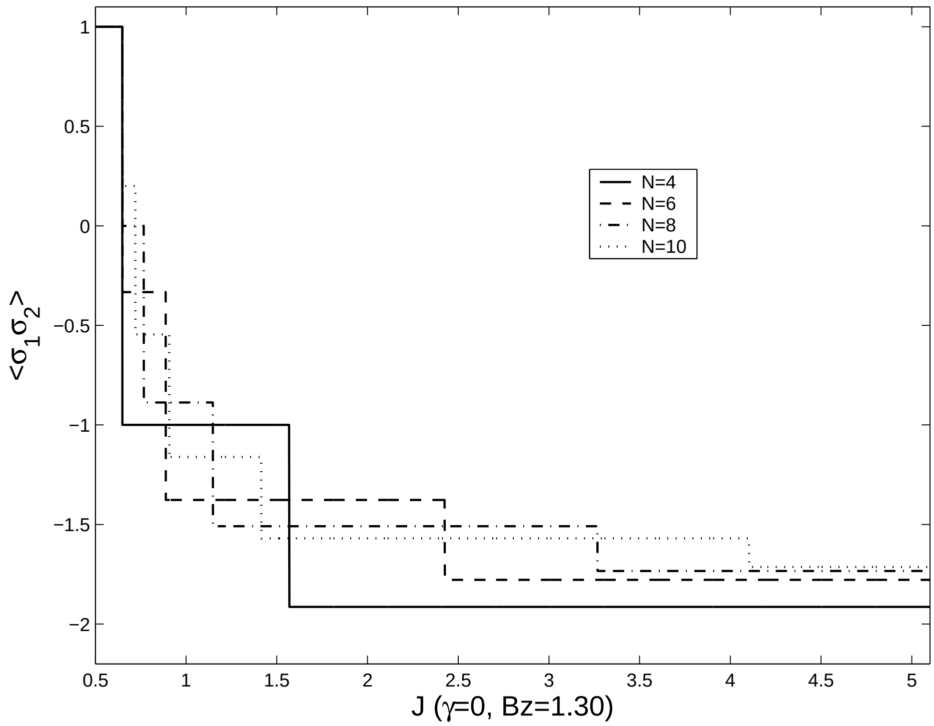


FIG. 1:

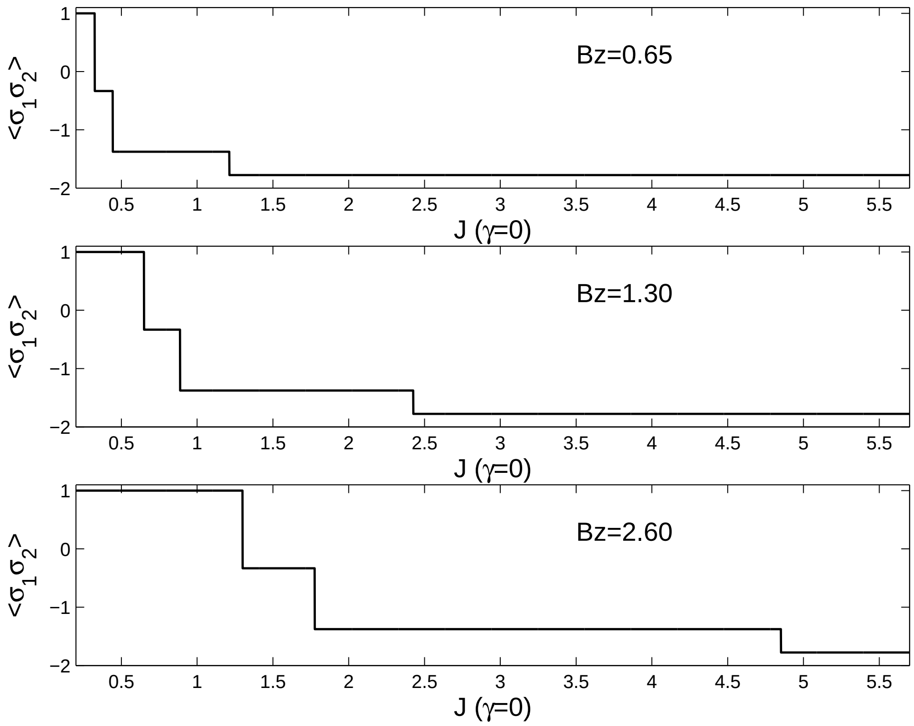
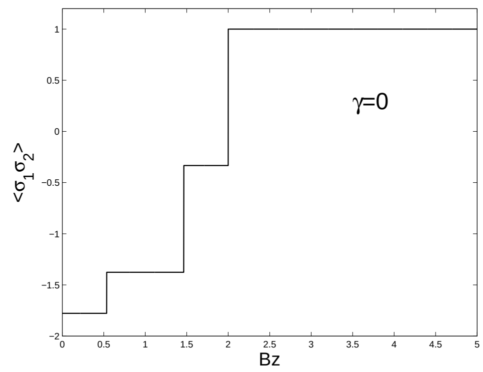
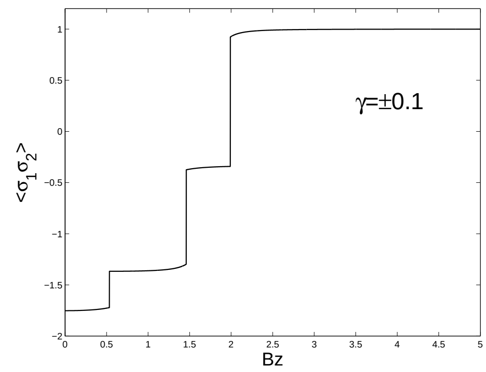


FIG. 2:



(a)$J = 1.0, \gamma = 0$



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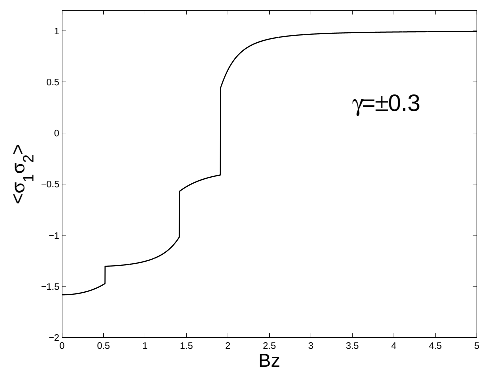
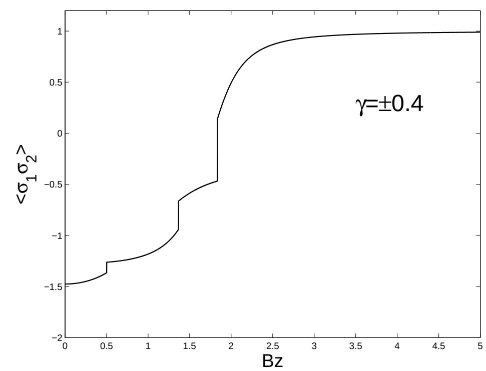
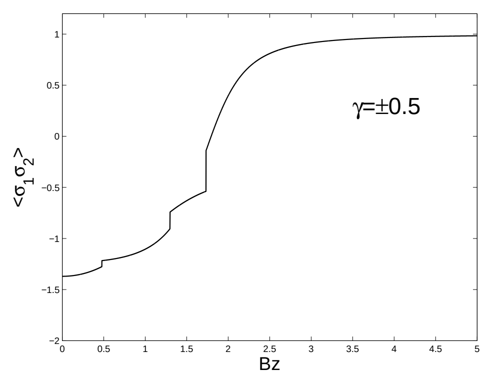


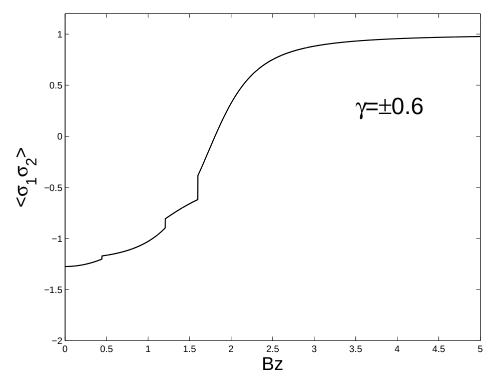
(c)$J = 1.0, |\gamma| = 0.3$



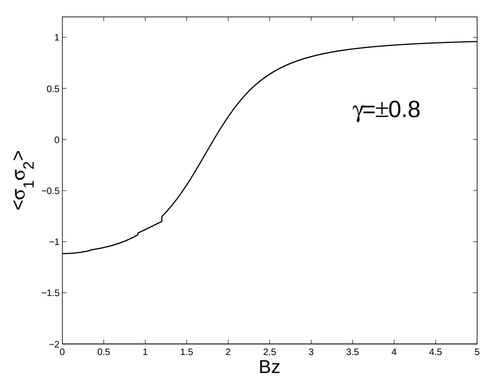
(d)$J = 1.0, |\gamma| = 0.4$



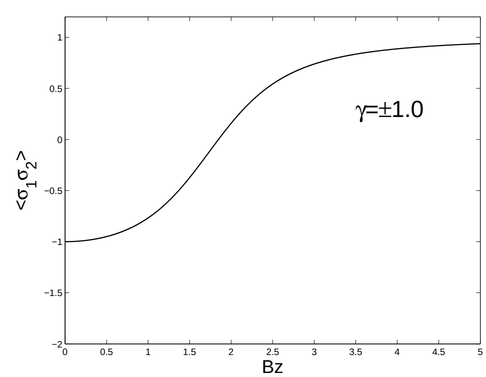
(e)$J = 1.0, |\gamma| = 0.5$



(f)$J = 1.0, |\gamma| = 0.6$



(g)$J = 1.0, |\gamma| = 0.8$



(h)$J = 1.0, |\gamma| = 1.0$

FIG. 3:

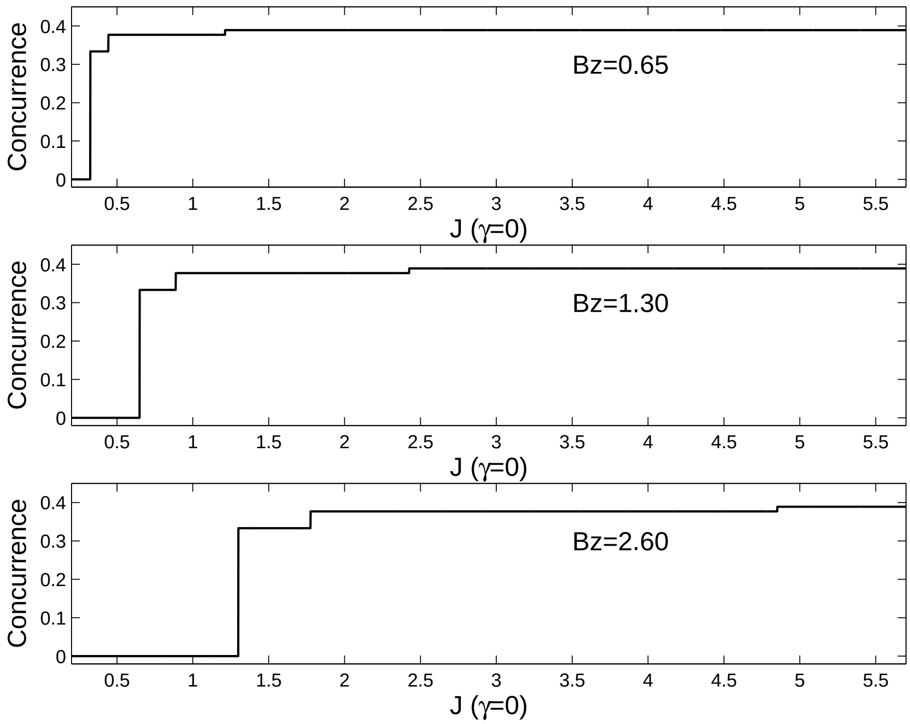
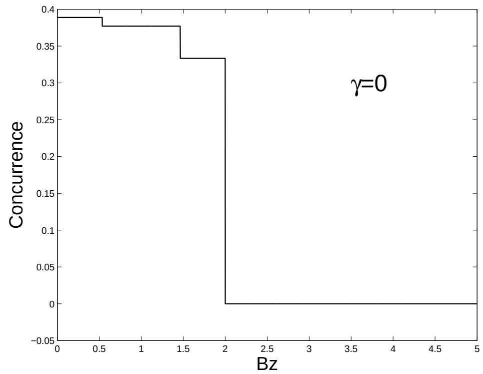
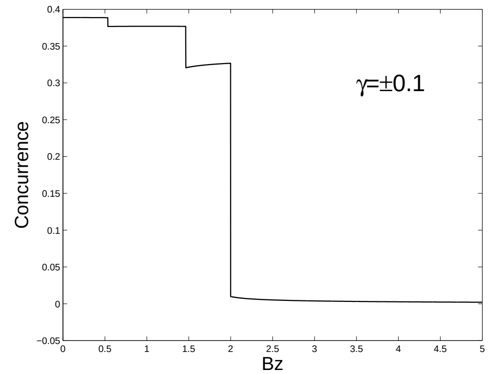

Concurrence
Bz=0.65
J (γ=0)
Concurrence
Bz=1.30
J (γ=0)
Concurrence
Bz=2.60
J (γ=0)

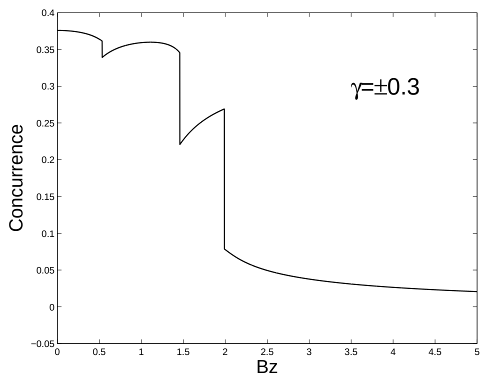
FIG. 4:



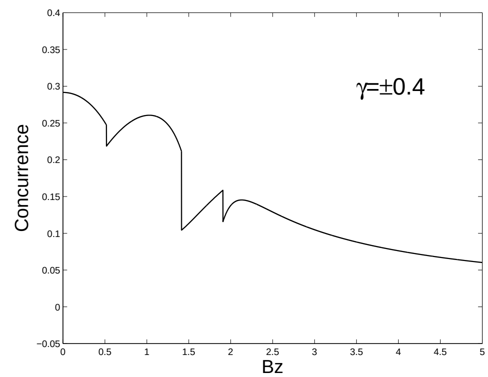
(a)$J = 1.0, \gamma = 0$



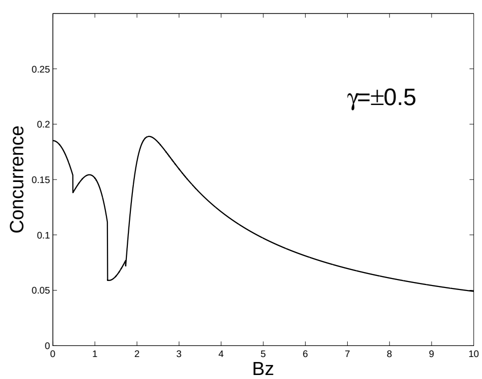
(b)$J = 1.0, |\gamma| = 0.1$



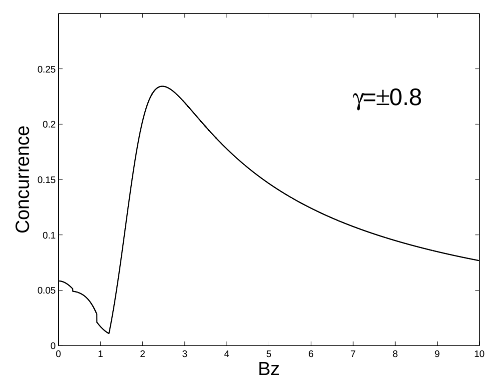
(c)$J = 1.0, |\gamma| = 0.3$



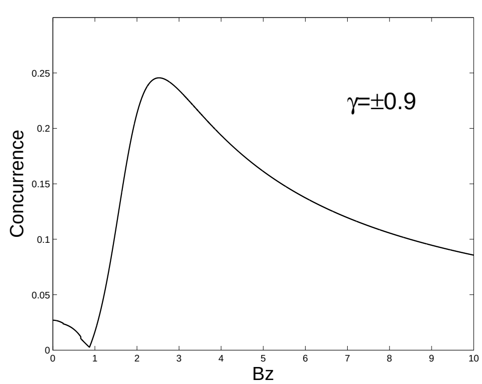
(d)$J = 1.0, |\gamma| = 0.4$



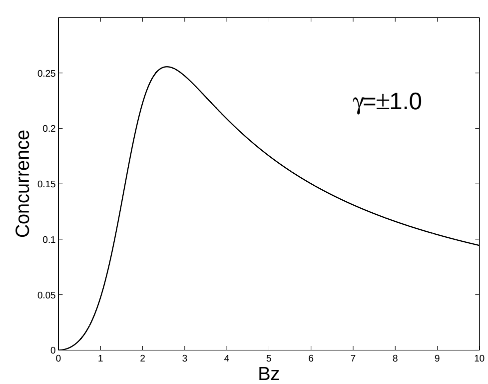
(e)$J = 1.0, |\gamma| = 0.5$



(f)$J = 1.0, |\gamma| = 0.8$



(g)$J = 1.0, |\gamma| = 0.9$



(h)$J = 1.0, |\gamma| = 1.0$

FIG. 5:

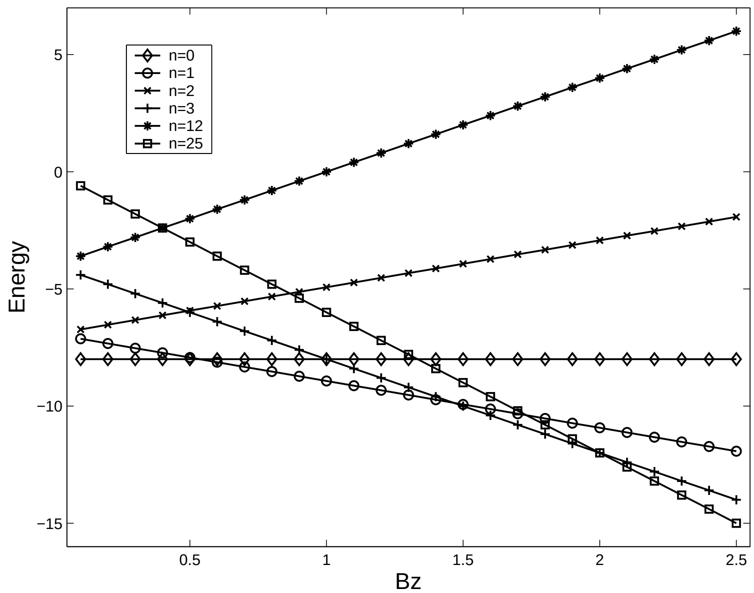
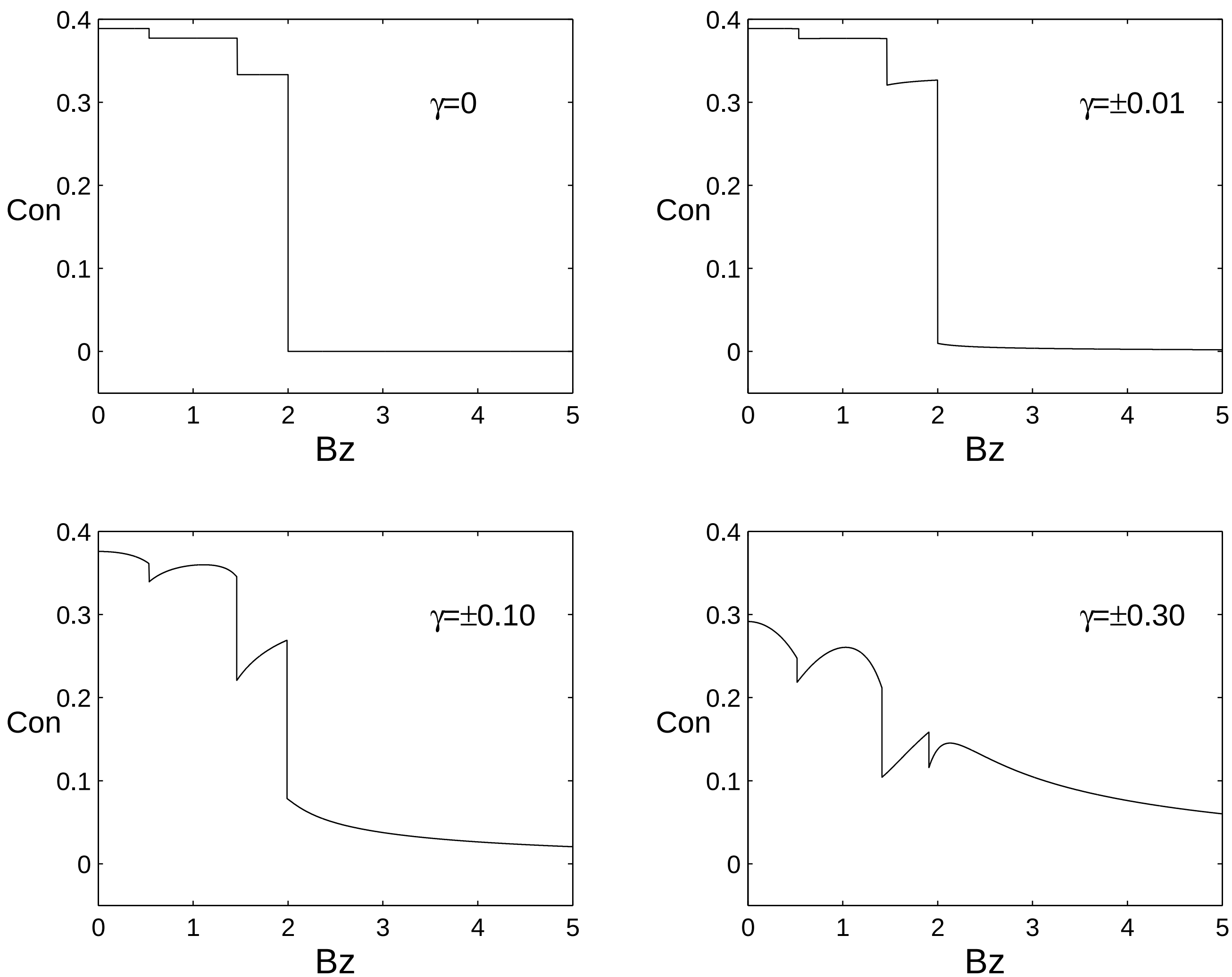
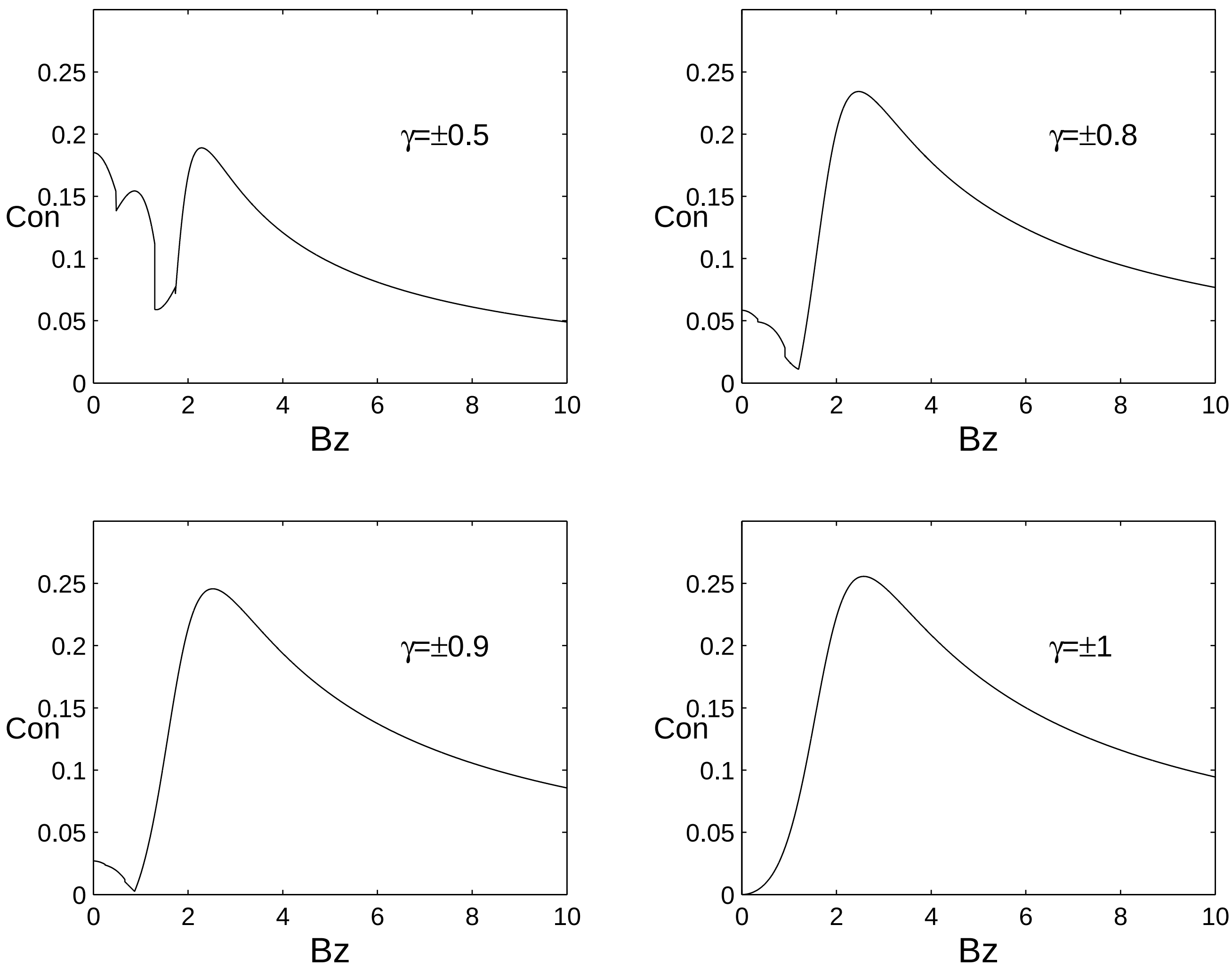


FIG. 6:



γ=0
γ=±0.01
γ=±0.10
γ=±0.30
Con
Bz
0.4
0.3
0.2
0.1
0
0
1
2
3
4
5



γ=±0.5
γ=±0.8
γ=±0.9
γ=±1
Con
Bz
0
0.05
0.1
0.15
0.2
0.25
2
4
6
8
10